

Magnetic dichroism in core-level photoemission from fcc Fe/Cu(100) films

D. P. Pappas

Naval Research Laboratory, Washington, DC 20375

G. D. Waddill and J. G. Tobin

Lawrence Livermore National Laboratory, Livermore, California 94550

Circularly polarized x rays from a synchrotron light source were used in photoemission from thin fcc Fe films on Cu(100). The measured exchange splitting for the $3s$ and $2p$ levels in these films is reduced from that measured in bulk bcc Fe. For both the $2p_{3/2}$ and the $2p_{1/2}$ levels the splittings are about half that of bulk bcc Fe. This trend is in line with measurements of the $3s$ exchange splitting from fcc Fe compared to bcc Fe as well. A 0.25 eV exchange splitting is observed in the $3p$ core level.

The difference in photoemission spectra for left versus right circularly polarized radiation (i.e., circular dichroism) can allow for a direct identification of the spin character of core-level states in magnetic samples.¹⁻³ Baumgarten *et al.*¹ have recently exploited this advantage of magnetic circular dichroism in photoemission (MCDPE) to deconvolute the exchange split $2p_{3/2}$ and $2p_{1/2}$ core levels in bulk single-crystal bcc Fe samples. This experiment confirmed that the unusually broad L_2 and L_3 lines do indeed contain contributions from exchange split lines.⁴ While it is still not possible to identify the direct cause of the line splitting (i.e., as a ground-state property of the system versus an exchange interaction of the photoelectron with the photohole) it is clear that this MCDPE gives similar information as, for example, spin-resolved photoemission (SRPE). However, with MCDPE only a factor of 10 loss of intensity is given up to obtain highly circularly polarized light,⁵ while SRPE entails the use of an electron spin detector, with typical efficiencies of 10^{-4} .⁶ In addition, the inherent surface sensitivity and elemental specificity of photoemission makes the study of the core-level splittings of very thin Fe films (2–4 atomic layers, AL) possible.

The magnetism and structure of thin Fe films grown on Cu(100) is interesting from a more general perspective. The lattice constant of the high-temperature, antiferromagnetic, fcc phase of Fe (γ -Fe) matches closely to that of Cu (3.59 vs 3.61 Å at room temperature),⁷ and it has been shown that fcc Fe does grow on the various Cu crystalline faces up to ≈ 10 AL. However, thin fcc Fe films grown on Cu(100) show distinct reconstructions as observed by low-energy electron diffraction (LEED),⁸ and also exhibit ferromagnetism with a strong surface anisotropy.⁹ We therefore chose MCDPE in order to compare the core-level splittings of the metastable, fcc Fe with those of bcc Fe.

In order to preserve the integrity of the Fe-Cu interface, the Fe layers were grown on a Cu(100) substrate at 150 K.¹⁰ A subsequent anneal to 300 K was then used to order the film. The LEED pattern sharpened significantly after the anneal, with the 5×1 reconstruction that is characteristic of thin fcc Fe layers grown at room temperature.

Following the deposition, the films were magnetized with up to 3 kOe pulses normal to the plane of the film. All measurements were made in remanence. Due to the strong surface anisotropy, the easy axis magnetization is perpendicular to the plane of the film for 2–6 AL thicknesses, and a single domain state has also been observed for this thickness range.^{11,12} Other specifics of the sample preparation and characterization can be found elsewhere.¹³

Circularly polarized radiation was obtained using a spherical grating monochromator at the Stanford Synchrotron Radiation Laboratory. When the photon helicity and sample magnetization are oriented parallel versus antiparallel the relative intensity of the spin-orbit split $2p$ core levels (the $2p_{3/2}$ and the $2p_{1/2}$ lines) changes. This is illustrated in Fig. 1. A slight change in binding energy of the two lines is also observed, which represents the exchange splitting of these lines. A simple explanation for the intensity variation and the shifts is presented in Ref. 1, while more quantitative theoretical descriptions are presented in Refs. 2 and 14.

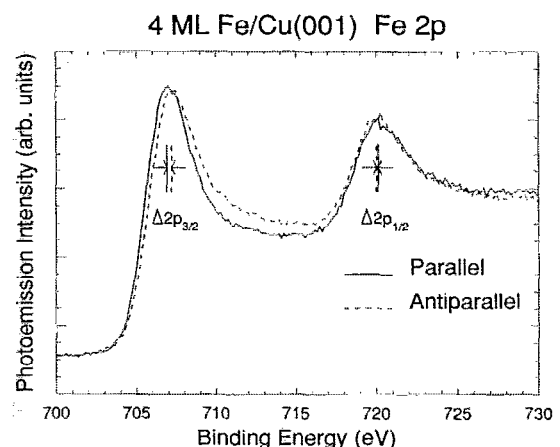


FIG. 1. Fe $2p$ spectra taken with $h\nu = 900$ eV and positive photon helicity. The solid lines are for parallel orientation of the photon helicity and sample magnetization and the dashed are for an antiparallel orientation.

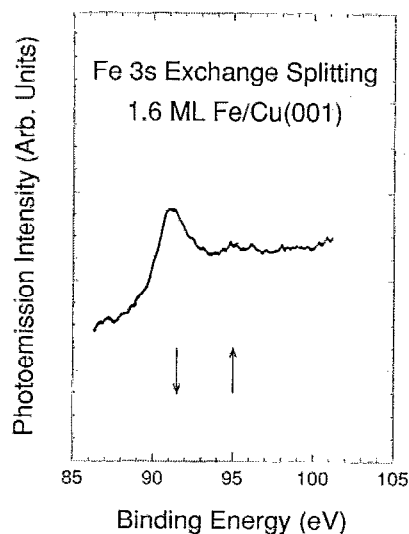


FIG. 2. Angle-resolved photoemission spectra of the fcc Fe 3s core level with $h\nu=190$ eV. The splitting is ≈ 3.8 eV.

In this paper we focus on the magnitude of the exchange splittings of the core-level lines of the thin fcc Fe films in comparison with those of bcc Fe. We obtain values for the exchange splittings of 0.22 ± 0.10 eV in the $2p_{3/2}$ level and 0.1 ± 0.1 eV in the $2p_{1/2}$ level from nonlinear least-square fits averaged over several sets of data similar to those presented in Fig. 1. These values are substantially smaller than those measured from bcc Fe, i.e., 0.5 ± 0.2 and 0.3 ± 0.2 in the $2p_{3/2}$ and the $2p_{1/2}$ lines, respectively.¹ We note here that the net moment on the fcc Fe films has been estimated by several techniques^{12,15} to be the same as that of bcc Fe, showing that there is not necessarily a linear relation between the moment at an atomic site and the core-level exchange splitting as observed by MCDPE.

The trend toward reduced exchange splitting of the fcc Fe core levels is also seen in the 3s and line.¹⁶ In Fig. 2 we

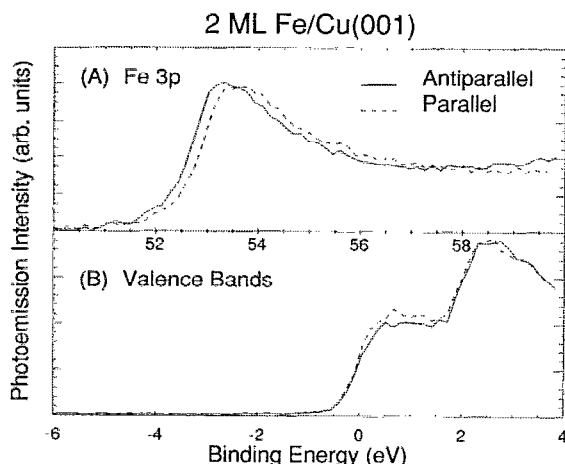


FIG. 3. Magnetic circular dichroism in photoemission of the fcc Fe 3p core level. The bottom panel shows the alignment of the Fermi edge, which allows for a direct comparison of the 3p binding energies in the top panel.

show the Fe 3s photoemission spectra from a 1.6 AL fcc Fe/Cu(100) film. The up and down arrows indicated the peak positions for the minority and majority electrons, respectively. A difference of 3.8 eV is measured, in contrast to the 4.4 eV splitting seen in bcc Fe.¹⁷

Finally, we present in Fig. 3 the first study of the fcc Fe 3d and 3p core levels with MCDPE. In the lower panel we show the alignment of the Fermi edges for the parallel and antiparallel alignments of photon helicity and magnetization. This alignment assures us that the core-level binding energy shifts are not artifacts due to, e.g., a systematic deflection of the electrons in the energy analyzer when the sample is magnetized. In the upper panel of Fig. 3 the MCDPE spectra from the Fe 3p core levels are shown. The same arguments used for the 2p core level are applicable in principle to the 3p states; however, the 3p spin-orbit splitting cannot be resolved experimentally. Thus, extraction of the exchange splitting is not as straightforward as in the 2p case. Nevertheless, SRPE¹⁸ has demonstrated that the minority spin energy distribution in the bcc Fe 3p manifold is concentrated at slightly lower binding energy (by about 0.5 eV) than the majority spin contribution. Assuming that the 3p spectra are predominantly weighted by the $3p_{3/2}$, we obtain a splitting of ≈ 0.25 eV, which again is about a factor of 2 smaller than SRPE results from bcc Fe. To date there have been no MCDPE studies of the bcc Fe 3p core level to compare our results with on an equal footing.

In conclusion, we find that the 2p and core-level splittings in fcc Fe are nearly a factor of 2 smaller than those of bcc Fe, while the 3s splitting from the fcc films is $\approx 86\%$ of the bcc Fe 3s splitting. We have also measured the fcc Fe 3p MCDPE spectrum, and find that the exchange splitting is also reduced when compared to SRPE studies of bcc Fe.

ACKNOWLEDGMENTS

This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract No. W-7405-ENG-48. Measurements were performed at the Stanford Synchrotron Radiation Laboratory, which is supported by the Department of Energy, Office of Basic Energy Sciences. The support of the SSRL staff is greatly appreciated. The work of D. P. P. was supported in part by IBM Almaden Research Center. We would also like to thank J. Stöhr and D. Weller for providing magnetic multilayer samples used to characterize the photon polarization.

¹ L. Baumgarten, C. M. Schneider, H. Petersen, F. Schäfers, and J. Kirschner, *Phys. Rev. Lett.* **65**, 492 (1990).

² G. van der Laan, *Phys. Rev. Lett.* **66**, 2527 (1991).

³ G. D. Waddill, J. G. Tobin, and D. P. Pappas, *Phys. Rev. B* **46**, 552 (1992).

⁴ J. C. Fuggle and S. Alvarado, *Phys. Rev. A* **22**, 1615 (1980).

⁵ C. T. Chen, F. Sette, Y. Ma, and S. Modesti, *Phys. Rev. B* **42**, 7262 (1990).

⁶ *Polarized Electrons in Surface Physics*, edited by R. Feder (World Scientific, Singapore, 1985).

⁷ S. H. Lu, J. Quinn, D. Tian, F. Jona, and P. M. Marcus, *Surf. Sci.* **209**, 364 (1989).

- ⁸W. Daum, C. Stuhlman, and H. Ibach, Phys. Rev. Lett. **60**, 2741 (1988).
- ⁹B. Heinrich, J. F. Cochran, A. S. Arrott, S. T. Purcell, K. B. Urquhart, J. R. Dutcher, and W. F. Egelhoff, Appl. Phys. A **49**, 473 (1989).
- ¹⁰D. A. Steigerwald, I. Jacob, W. F. Egelhoff, Jr., Surf. Sci. **202**, 472 (1988).
- ¹¹C. Liu, E. R. Moog, and S. D. Bader, Phys. Rev. Lett. **60**, 2422 (1988).
- ¹²D. P. Pappas, C. R. Brundle, and H. Hopster, Phys. Rev. B **45**, Rapid Communication, 8169 (1992).
- ¹³D. P. Pappas, *Magnetism of Ultra-thin Films of Fe on Cu(100)* (University Microfilms, Ann Arbor, MI) No. 91-09652.
- ¹⁴B. T. Thole and G. van der Laan, Phys. Rev. Lett. **67**, 3306 (1991).
- ¹⁵W. Schwarzacher, W. Allison, R. F. Willis, J. Penfold, R. C. Ward, I. Jacob, and W. F. Egelhoff, Jr., Solid State Commun. **71**, 563 (1989).
- ¹⁶J. G. Tobin, M. K. Wagner, X.-Q. Guo, and S. Y. Tong, Mater. Res. Soc. Symp. Proc. **208**, 283 (1991).
- ¹⁷C. S. Fadley and D. A. Shirley, Phys. Rev. A **2**, 1109 (1970).
- ¹⁸Carbone and E. Kisker, Solid State Commun. **64**, 1107 (1988).